PBE						
molecule	Total Energy [a.u.]		molecule	dissociation energy [kcal/mol]		
	CP2K	ADF		CP2K	ADF	Reference
CH3	-7.40469	-0.66649	CH3-CH3	92.59	404.84	96.79
OCH3	-23.41905	-0.89946	CH3-OCH3	81.48	86.95	87.24
isopropyl	-21.18145	-1.89197	CH3-isopropyl	86.01	89.76	89.65
CH3-CH3	-14.95634	-1.97559	OCH3-isopropyl	77.69		84.08
CH3-OCH3	-30.95307	-1.70397				
Isopropyl-CH3	-28.72266	-2.70094				
Isopropyl-OCH3	-44.72382	running				